# Spermine, tetrakis-MOC derivative

**Inchi:** InChI=1S/C16H32N4O6/c1-24-14(21)18-10-6-9-17-8-4-5-12-20(16(23)26-3)13-7-11-19-1
**InchiKey:** QZHZSQNMWZRHNY-UHFFFAOYSA-N
**Formula:** C16H32N4O6
**SMILES:** COC(=O)NCCCNCCCCN(CCCNC(=O)OC)C(=O)OC
**Mol. weight [g/mol]:** 376.45

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -238.97 | kJ/mol | Joback Method |
| hf | -880.03 | kJ/mol | Joback Method |
| hfus | 63.87 | kJ/mol | Joback Method |
| hvap | 100.03 | kJ/mol | Joback Method |
| log10ws | -2.18 | | Crippen Method |
| logp | 0.917 | | Crippen Method |
| mcvol | 298.540 | ml/mol | McGowan Method |
| pc | 1503.48 | kPa | Joback Method |
| rinpol | 3055.00 | | NIST Webbook |
| tb | 957.30 | K | Joback Method |
| tc | 1172.50 | K | Joback Method |
| tf | 677.01 | K | Joback Method |
| vc | 1.127 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1000.49 | J/mol×K | 957.30 | Joback Method |
| cpg | 1013.69 | J/mol×K | 993.17 | Joback Method |
| cpg | 1025.47 | J/mol×K | 1029.03 | Joback Method |
| cpg | 1035.87 | J/mol×K | 1064.90 | Joback Method |
| cpg | 1044.88 | J/mol×K | 1100.77 | Joback Method |
| cpg | 1052.54 | J/mol×K | 1136.63 | Joback Method |
| cpg | 1058.85 | J/mol×K | 1172.50 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R333747&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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